

First-passage time: Lattice versus continuum

Kamal Sharma and N. Kumar

Raman Research Institute, Bangalore 560080, India

(Received 2 May 2012; revised manuscript received 20 July 2012; published 11 September 2012)

The well known approach, based on Schrödinger's integral equation, to the problem of calculating the first-passage probability density in time for classical diffusion on a continuum is revisited for the case of diffusion by hopping on a discrete lattice. It turns out that a certain boundary condition central to solving the integral equation, invoked first by Schrödinger and then by others on the basis of a physical argument, needs to be modified for the discrete case. In fact, the required boundary condition turns out to be determined entirely by the normalization condition for the first-passage probability density. An explicit analytical expression is derived for the first-passage density for a three-site problem modeling escape over a barrier. The related quantum first-passage problem is also commented upon briefly.

DOI: [10.1103/PhysRevE.86.032104](https://doi.org/10.1103/PhysRevE.86.032104)

PACS number(s): 02.50.-r, 03.65.-w, 06.30.Ft

For any physical event, there is necessarily a time of its first passage past the post, i.e., a marker [1–4]. For a randomly occurring event, therefore, one must speak of the calculable probability density in time of its first passage. The robustness of this elementary notion can hardly be questioned—certainly classically, but possibly even quantum mechanically [4,5]. Its conceptual significance in the context of time in quantum mechanics [6] aside, the first-passage probability density is also of considerable physical interest, e.g., for catalysis or barrier crossing [6,7]. Thus, e.g., a chemical reaction involving classical escape over a barrier along the reaction coordinate should necessarily be dominated by the first passage past the post (the barrier), rather than by the mean Kramers rate [8].

The problem of the first-passage probability density in time was addressed and solved by Schrödinger [1] (almost ten years before the appearance of his wave equation) for the special case of classical diffusion on a one-dimensional (1D) continuum, $-\infty < x < \infty$. He obtained the first-passage probability density as the solution of a physically transparent integral equation [1,3,4],

$$\begin{aligned} \phi_u(x \leq B, t | A, 0) &= \phi_r(x \leq B, t \geq t' \geq 0 | A, 0) \\ &+ \int_0^t -\frac{\partial}{\partial t'} \phi_r(x \leq B, t \geq t' \geq 0 | A, 0) \\ &\times \phi_u(x \leq B, t | B, t') dt', \end{aligned} \quad (1)$$

with $\phi_u(x \leq B, t | B, t')$ a function of $(t - t')$. Here, $\phi_u(x \leq B, t | A, 0)$ denotes *unrestricted* (u) probability that the particle initially ($t = 0$) at position $x = A$ is found at the later time ($t > 0$) in the interval $x \leq B$; $\phi_r(x \leq B, t \geq t' \geq 0 | A, 0)$ is the *restricted* (r) probability that the particle initially at $x = A$ remains confined to $x \leq B$ for all times $t' \leq t$; and $\phi_u(x \leq B, t | B, t')$ is the *unrestricted* probability that the particle at the post B at time t' is found to lie in the space $x \leq B$ at time $t (> t')$. Then $-\frac{\partial}{\partial t'} \phi_r(x \leq B, t \geq t' \geq 0 | A, 0) \equiv P_{(\text{IPT})}^C(t')$ is clearly the classical probability density of first-passage time past the post (i.e., marker) $x = B$ at time t' . Now, the integral equation (1) had to be supplemented by the boundary condition

$$\phi_u(x \leq B, t | B, t') \rightarrow \frac{1}{2} \quad \text{for } t - t' \rightarrow 0^+. \quad (2)$$

This followed from the physical condition that the diffusing particle arriving at the post $x = B$ at time t is equally likely to make the first move to the left or to the right. The integral equation (1) can then be readily solved by taking its time-Laplace transform (and remembering that the Laplace transform of a convolution of two functions is the product of their Laplace transforms). The resulting solution was in agreement with the one obtained by using the theoretical device of a perfect absorber and the Kelvin method of images [2].

In this Brief Report, we have revisited the classical first-passage problem, but now for the case of diffusion by hopping on a *discrete lattice* rather than on a *1D continuum*. This is with a view to reexamining the stated boundary condition as in Eq. (2), invoked crucially in Schrödinger's integral Eq. (1). The essential difference between the two cases is the following: For the discrete case, the first-passage event also involves a time of *sojourn* at the marker site (the post) separating the instant of arrival at that site and the instant of its departure from that site. The idea of such a *sojourn time at-a-point on a continuum* is, however, physically meaningless. This finer subdivision of the first-passage event (or rather its disambiguation with respect to arrival, sojourn, and departure) alters the boundary condition for the Schrödinger integral equation for the discrete lattice case in a nontrivial manner. We demonstrate this explicitly for a three-site problem that can model the canonical Kramers escape over the barrier. The boundary condition turns out to be uniquely determined by the condition of normalization of the first-passage probability density—in fact, in the three-site problem, Schrödinger's half (1/2) gets replaced by unity (1). We also comment briefly on the quantum first-passage problem in this context.

Consider the diffusive motion of a *particle* by classical nearest-neighbor hopping over a three-site finite lattice ABC as shown schematically in Fig. 1. Here, the site B represents the barrier (the post) separating the reaction coordinate A (for reactants) and the reaction coordinate C (for the reaction products).

We are interested in the first-passage probability density in time for the *particle* initially at A . The diffusion by random hoppings is described by the master equation for the site

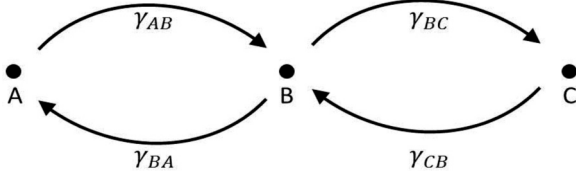


FIG. 1. A model three-site problem for classical diffusion by hopping on a discrete space. The γ 's are the hopping probability rates.

probabilities $p_A(t)$, $p_B(t)$, and $p_C(t)$:

$$\frac{dp_A(t)}{dt} = -\gamma_{AB}p_A(t) + \gamma_{BA}p_B(t), \quad (3a)$$

$$\frac{dp_B(t)}{dt} = -(\gamma_{BA} + \gamma_{BC})p_B(t) + \gamma_{AB}p_A(t) + \gamma_{CB}p_C(t), \quad (3b)$$

$$\frac{dp_C(t)}{dt} = -\gamma_{CB}p_C(t) + \gamma_{BC}p_B(t). \quad (3c)$$

The various *unrestricted* probabilities, such as $\phi_u(x \leq B, t | A, 0)$ and $\phi_u(x \leq B, t | B, t')$, that enter the integral equation (1) can be derived straightforwardly from the above Eqs. (3a)–(3c), with appropriate initial/boundary conditions. It is convenient to rewrite these equations in terms of their

Laplace transforms as

$$\begin{pmatrix} (s + \gamma_{AB}) & -\gamma_{BA} & 0 \\ -\gamma_{AB} & (s + \gamma_{BA} + \gamma_{BC}) & -\gamma_{CB} \\ 0 & -\gamma_{BC} & (s + \gamma_{CB}) \end{pmatrix} \begin{pmatrix} \tilde{p}_A(s) \\ \tilde{p}_B(s) \\ \tilde{p}_C(s) \end{pmatrix} = \begin{pmatrix} p_A(0) \\ p_B(0) \\ p_C(0) \end{pmatrix}, \quad (4)$$

with $\tilde{p}_A(s) = \int_0^\infty e^{-st} p_A(t) dt$, etc., and $p_A(0)$, etc., the corresponding initial/boundary conditions.

Now, in order to obtain the unrestricted probability $\phi_u(x \leq B, t | A, 0)$, we must solve Eq. (4) for $\tilde{p}_A(s)$ and $\tilde{p}_B(s)$ with the initial/boundary conditions $p_A(0) = 1$ and $p_B(0) = 0 = p_C(0)$. And similarly, for the case of *unrestricted* probability $\phi_u(x \leq B, t | B, t')$, we must solve Eq. (4) for $\tilde{p}'_A(s)$ and $\tilde{p}'_B(s)$ with the initial/boundary conditions $p'_A(0) = 0 = p'_C(0)$, but $p'_B(0) = X$. (The prime denotes the “X” boundary conditions.) As will be shown below, the unknown X will eventually be determined by the normalization condition for the first-passage probability density in time, $P_{\text{IPT}}^C(t)$.

After some tedious but straightforward algebra, we obtain from Eqs. (1), (3), and (4) the classical first-passage probability density [its Laplace transform $\tilde{P}_{\text{IPT}}^C(s)$] as

$$\tilde{P}_{\text{IPT}}^C = \frac{1 - s[\tilde{p}_A(s) + \tilde{p}_B(s)]}{1 - s[\tilde{p}'_A(s) + \tilde{p}'_B(s)]} \quad (5a)$$

$$= \frac{\Delta[\gamma_{AB}s(\gamma_{CB} + s) - 1] + s[\gamma_{BA}(\gamma_{CB} + s) + s(\gamma_{BC} + \gamma_{CB} + s)]}{Xs(\gamma_{CB} + s)[\Delta(\gamma_{AB} + s) + \gamma_{BA}] - \Delta}. \quad (5b)$$

Here the determinant

$$\Delta = s[\gamma_{AB}(\gamma_{BC} + \gamma_{CB} + s) + \gamma_{BA}(\gamma_{CB} + s) + s(\gamma_{BC} + \gamma_{CB} + s)]. \quad (5c)$$

The unknown boundary condition parameter X is now readily determined from the normalization condition:

$$\tilde{P}_{\text{IPT}}^C(s) \rightarrow 1 \quad \text{as } s \rightarrow 0, \quad (6a)$$

giving the unique solution

$$X = 1, \quad (6b)$$

and not $1/2$ as for the continuum case. [In deriving the condition (6b), it is necessary to keep, as $s \rightarrow 0$, the leading nonvanishing terms in the numerator/denominator on the right-hand side of Eq. (5b), and these turn out to be of higher-order in s .] The $P_{\text{IPT}}^C(t)$ turns out to be

$$P_{\text{IPT}}^C(t) = \gamma_{AB} \exp(-\gamma_{AB}t). \quad (6c)$$

Note that $P_{\text{IPT}}^C(t)$ depends only on γ_{AB} for the three-site problem. This result of ours, namely that the classical first-passage time probability density $P_{\text{IPT}}^C(t)$ turns out to be independent of γ_{BC} , is indeed somewhat puzzling—more so in the limit of $\gamma_{BC} \rightarrow 0$, when the passage past the post B is clearly not possible. This can, however, be physically understood in terms of the essential difference between a

spatial continuum and the discrete three-site case considered here. Indeed, as pointed out earlier, unlike the case for spatial continuum, where the particle arriving at the point (post) has to necessarily move on to the right or to the left, in our discrete case it can also have a finite sojourn time at the lattice site in question. (For a spatial continuum, a finite sojourn-at-a spatial point is physically inadmissible under the diffusive motion.) Thus, for our three-site discrete case, the first-passage time becomes effectively the time of first arrival at the site (the post), which may be followed by a finite sojourn time at that site without having to make an immediate passage past that site.

In Fig. 2, we have plotted the classical first-passage probability density in time $P_{\text{IPT}}^C(t)$ for the three-site problem for a certain choice of parameters γ_{AB} , etc. We note that $P_{\text{IPT}}^C(t)$ remains positive and is normalized.

Finally, some comments are in order on the related question of quantum (Q) first-passage time problem—the possibility of calculating the $P_{\text{IPT}}^Q(t)$. The classical approach based on the Schrödinger integral equation, or equivalently using a theoretical device such as a perfect absorber placed at the post

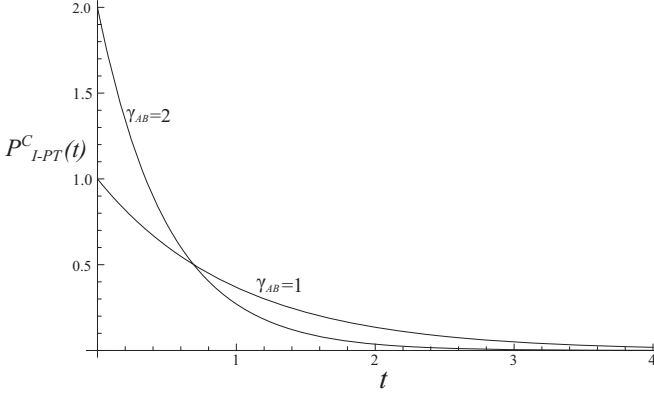


FIG. 2. Plot of the classical first-passage probability density in time $P_{\text{LPT}}^C(t) = \gamma_{AB} \exp(-\gamma_{AB}t)$ for some typical parameter values chosen: $\gamma_{AB} = 1$ and 2.

(the marker), does not generalize directly to the quantum case. This can be appreciated best by considering the classical (C) diffusion and its quantum (Q) counterpart for a 1D continuum:

$$\frac{\partial}{\partial t} P^C(x,t) + \frac{\partial}{\partial x} j^C(x,t) = 0, \quad (7a)$$

with the classical probability current $j^C(x,t) = -D \frac{\partial}{\partial x} P^C(x,t)$, and

$$\frac{\partial}{\partial t} P^Q(x,t) + \frac{\partial}{\partial x} j^Q(x,t) = 0, \quad (7b)$$

with the quantum probability current $j^Q(x,t) = -\frac{\hbar}{m} P^Q(x,t) \frac{\partial \theta}{\partial x}$, where $P^Q(x,t) = \psi^*(x,t)\psi(x,t)$ and $\psi(x,t) = [P^Q(x,t)]^{1/2} e^{i\theta}$ in obvious notation. The two cases do have a formal similarity. Also, stochastic processes underlie both of these physical diffusions—the Wiener process for the classical diffusion, determining random trajectories with associated path *probabilities* (real), and the Feynman-Kac process for the quantum case with the associated path-probability *amplitudes* (complex). The essential difference, however, is that while the random trajectories underlying the classical diffusion are real and can in principle be tracked continuously without affecting them, the quantum paths are virtual and cannot be tracked even in principle without affecting (collapsing) them. Thus, it is not clear how to treat the *virtual excursions* past the post (B) in describing, e.g., the restricted (r) probabilities in the Schrödinger integral equation (1)—one has the problem of interference between these virtual paths and the restricted paths contributing to the probability $\phi_r(x \leq B, t \geq t' \geq 0 | A, 0)$ in Eq. (1). One could argue, though, in favor of envisaging a *weak measurement* of the virtual excursions here (possibly through a weak coupling to a fluctuating dissipating degree of freedom [4], or by introducing suitable Lindblads [9]), or attempt a strictly quantum restricted path-decomposition approach [10,11]; however, this remains to be worked out in detail. The difference between the classical and the quantum case is brought into sharp focus when we use the theoretical device of a *perfect absorber* that instantaneously absorbs the particle upon approaching the post (and thus removes it from view). For classical diffusion, this simply means setting

$P^C(x = B, t) = 0$ for all times t . The classical probability current $j^C(x = B, t)$ may, however, remain nonzero and positive. This leakage allows for the removal of the particle by the perfect absorber placed at the post B. All one has to do, therefore, is to solve the classical diffusion problem with the boundary condition of vanishing probability density at $x = B$, and obtain $P_{\text{LPT}}^C(B, t) = -\frac{\partial}{\partial t} \int_{-\infty}^B P^C(x, t) dx$. This clearly fails in the quantum case. As can be seen from Eq. (7b), a perfect absorber placed at the post, of course, does make $P^Q(x = B, t) = 0$ at the boundary, but concomitantly it also makes the probability current $j^Q(B, t)$ vanish—there is no absorption possible. Thus a *perfect absorber* becomes a *perfect reflector* too in the quantum case.

In conclusion, the Schrödinger integral equation for calculating the first-passage probability density in time on a 1D continuum requires a modification of the original boundary condition for the classical diffusion on a discrete lattice. This has been explicitly demonstrated here for the three-site problem, where Schrödinger's 1/2 gets replaced by 1. This has also been verified in the case of an infinite discrete lattice, where the boundary condition determined by the normalization condition again comes out to be unity (see the Appendix). Straightforward generalization to the quantum case remains essentially problematic.

The authors would like to thank the referee for very constructive comments, and for motivating us to further generalize our treatment for a nonuniform infinite lattice. One of us (K.S.) would like to thank the Raman Research Institute for support under its Visiting Student Programme (VSP) during the course of this work.

APPENDIX

Our treatment of the classical first-passage time for the three-site problem can be readily generalized to the case of an infinite lattice of sites. The diffusion by random hopping is now described by the master equation for the site (n) probability $p_n(t)$,

$$\dot{p}_n(t) = -2p_n(t) + p_{n-1}(t) + p_{n+1}(t), \quad (A1)$$

where we have set the nearest-neighbor transition rate $\gamma = 1$.

Introducing the time-Laplace and the lattice-Fourier transforms

$$\tilde{p}_n(s) = \int_0^\infty p_n(t) e^{-st} dt, \quad \tilde{\tilde{p}}(s, k) = \sum_{n=-\infty}^{+\infty} \tilde{p}_n(s) e^{ikn}, \quad (A2)$$

we obtain

$$s \tilde{\tilde{p}}(s, k) + 2 \tilde{\tilde{p}}(s, k) - 2 \cos k \tilde{\tilde{p}}(s, k) = \sum_{n=-\infty}^{+\infty} p_n(t=0) e^{ikn}. \quad (A3)$$

Here the overhead tilde and dash denote, respectively, the time-Laplace and the lattice-Fourier transform.

To solve for the classical first-passage time probability density $P_{\text{LPT}}^C(t)$, we need as before solutions of Eq. (A3) for

the two initial/boundary conditions, B and B' , with

$$\begin{aligned} B &: p_n(t=0) = \delta_{n,0} \\ &\Rightarrow \text{initially the particle is at site } n=0, \\ B' &: p'_n(t=0) = X\delta_{n,N} \\ &\Rightarrow \text{initially the particle is at site } n=N \text{ (the post)}. \end{aligned}$$

The constant X will be determined by the condition of normalization on $P_{\text{IPT}}^C(t)$. Note that the ‘‘prime’’ distinguishes between the two conditions B and B' as above. Also, we will take $N > 0$ without loss of generality.

With the unprimed condition B , the solution for $\tilde{p}(s,k)$ is

$$\tilde{p}(s,k) = \left(\frac{1}{s+2-2\cos k} \right). \quad (\text{A4})$$

Inverting the lattice Fourier transform, we obtain

$$\tilde{p}(s,n) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} \frac{1}{s+2-2\cos k} e^{-ikn} dk, \quad (\text{A5})$$

leading to the sum

$$\sum_{n=-\infty}^N \tilde{p}(s,n) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk \frac{1}{s+2-2\cos k} \left(\frac{e^{-ikN}}{1-e^{ik}} \right) dk, \quad (\text{A6})$$

which goes into the numerator of the expression corresponding to Eq. (5a) for $\tilde{P}_{\text{IPT}}^C(s)$ based on the Schrödinger integral equation.

Next, we consider the primed initial/boundary condition B' . Here we have

$$s\tilde{p}'(s,k) + 2\tilde{p}'(s,k) - 2\cos k\tilde{p}'(s,k) = X e^{ikN}, \quad (\text{A7})$$

giving

$$\tilde{p}'(s,k) = X \left(\frac{e^{ikN}}{s+2-2\cos k} \right). \quad (\text{A8})$$

Again, inverting the lattice Fourier transform, we obtain

$$\sum_{n=-\infty}^N \tilde{p}'(s,n) = \frac{X}{2\pi} \int_{-\pi}^{+\pi} dk \frac{1}{(s+2-2\cos k)(1-e^{ik})}. \quad (\text{A9})$$

This goes into the *denominator* of the expression corresponding to Eq. (5a) for $\tilde{P}_{\text{IPT}}^C(s)$ based on the Schrödinger integral equation.

Thus, we have

$$\begin{aligned} \tilde{P}_{\text{IPT}}^C(s) &= \frac{1-s \sum_{n=-\infty}^N \tilde{p}(s,n)}{1-Xs \sum_{n=-\infty}^N \tilde{p}'(s,n)} \\ &= \frac{1-s \frac{1}{2\pi} \int_{-\pi}^{+\pi} \frac{e^{-ikN}}{s+2-2\cos k} \left(\frac{1}{1-e^{ik}} \right) dk}{1-Xs \frac{1}{2\pi} \int_{-\pi}^{+\pi} \frac{dk}{s+2-2\cos k} \left(\frac{1}{1-e^{ik}} \right)}. \end{aligned} \quad (\text{A10})$$

Now, the integral over k can be converted into a contour integral in the complex z plane using $z = e^{ik}$, $dz = e^{ik} i dk$, and $-\pi \leq k \leq +\pi$. Finally, we obtain the desired expression

$$\tilde{P}_{\text{IPT}}^C(s) = \frac{1 - \frac{s}{2\pi i} \oint \frac{e^{-i(1+N)z} dz}{s+2-(z+\frac{1}{z})(\frac{1}{1-z})}}{1 - X \frac{s}{2\pi i} \oint \frac{dz}{z[s+2-(z+\frac{1}{z})(1-z)]}}. \quad (\text{A11})$$

The singularities relevant to the above contour integrals are the three simple poles z_0, z_{\pm} with

$$z_0 = 1, \quad z_{\pm} = 1 + \frac{s}{2} \pm \frac{\sqrt{s^2+4s}}{2}. \quad (\text{A12})$$

Clearly, only the pole z_- lying within the contour contributes to the integral. With this, we obtain

$$\tilde{P}_{\text{IPT}}^C(s) = \frac{1 + s \frac{(1+\frac{s}{2}-\frac{1}{2}\sqrt{s^2+4s})^{-(1+N)}}{(z_- - z_+)(1-z_-)}}{1 - X \frac{s(1-s^{1/2})}{(-2\sqrt{s})(s^{1/2})}}. \quad (\text{A13})$$

Now, for the normalization of the first-passage time probability density $P_{\text{IPT}}^C(t)$, we require that the limit $\tilde{P}_{\text{IPT}}^C(s \rightarrow 0) = 1$. Thus, we need the expression in (A13) for small $s (\rightarrow 0)$. This gives

$$\begin{aligned} \int_0^{\infty} P_{\text{IPT}}^C(t) dt &= \lim_{s \rightarrow 0} \tilde{P}_{\text{IPT}}^C(s) \\ &= \frac{1 + \frac{1 + \text{higher order in } s}{2 + \text{higher order in } s}}{1 + \frac{X(1 + \text{higher order in } s)}{2(1 + \text{higher order in } s)}}. \end{aligned} \quad (\text{A14})$$

This fixes the constant $X = 1$. This is exactly what we had obtained earlier for the three-site problem.

-
- [1] E. Schrödinger, *Phys. Z.* **16**, 289 (1915).
[2] W. Feller, in *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1950).
[3] A. J. F. Sigert, *Phys. Rev.* **81**, 617 (1951).
[4] O. Lumpkin, *Phys. Rev. A* **51**, 2758 (1995).
[5] S. Brouard, D. Macias, and Muga, *J. Phys. A* **27**, L439 (1994).
[6] J. G. Muga, R. Sals Mayato, and I. L. Egusquiza, *Time in Quantum Mechanics* (Springer, Berlin, 2002).

- [7] D. S. Wuttke, M. Bjerrum, J. R. Winkler, and H. B. Gray, *Science* **256**, 1007 (1992).
[8] S. Chandrasekhar, *Rev. Mod. Phys.* **15**, 1 (1943).
[9] J. J. Halliwell, [arXiv:quant-ph/9805057](https://arxiv.org/abs/quant-ph/9805057).
[10] A. Auerbach, S. Kivelson, and D. Nicole, *Phys. Rev. Lett.* **53**, 411 (1984).
[11] N. Kumar, *Pramana-J. Phys.* **25**, 363 (1985).